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# **TOWARD THE USE OF SIMILARITY THEORY IN TWO-PHASE CHOKED FLOWS**

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## **TOWARD THE USE OF SIMILARITY THEORY IN TWO-PHASE CHOKED FLOWS**

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### **ABSTRACT**

Comparison of two-phase choked flows in normalized coordinates were made between pure components and available data using a reference fluid to compute the thermophysical properties. The results are favorable. Solution of the governing equations for two LNG mixtures show some possible similarities between the normalized choked flows of the two mixtures, but the departures from the pure component locii are significant.

## NOMENCLATURE

$a_{1-5}$	constants, eq. (11)
$b_{1-4}$	constants, eq. (12)
$G$	mass flux ( $G = \rho U$ )
$G^*$	mass flux normalizing parameter ( $\sqrt{P_c \rho_c / Z_c}$ )
$G_a^*$	$(\sqrt{f/h})G_0^*$ for corresponding states with reference fluid (0) and working fluid (a)
$g$	configurational free energy
$h$	scaling function - volume
$f$	scaling function - temperature
$m$	molecular weight
$P$	pressure
$R$	gas constant
$S$	entropy
$T$	temperature
$U$	fluid velocity
$V$	specific volume
$x$	mole fraction
$Z$	compressibility

## Greek:

$\rho$	density
$\eta, \delta$	binary interaction parameter
$\phi$	configuration function
$\omega$	Pitzer's eccentric factor
$t$	property parameter

## Subscripts:

c	critical
e	exit
a	fluid-a
ij	fluid i - fluid j
o	reference fluid
m	mixture
t	throat
R	reduced

Superscript:	
c	critical

## INTRODUCTION

Using conventional corresponding states techniques, we have found normalizing parameters which can be applied in two-phase choked flow computations (refs. 1 to 4). The pure component properties of the working fluid, along with the flow equations, are used to define the critical mass flux and pressure ratio profiles. When compared to available experimental data the agreement was good (refs. 4 and 5).

Although the normalized charts are applicable to a wide variety of simple fluids, it has not been demonstrated, via direct calculation, that a reference fluid (0) can be used to predict the proper-

ties of another fluid ( $\alpha$ ) in conjunction with calculations of two-phased choked flow parameters for fluid ( $\alpha$ ) using fluid (0); the pure-pure problem.

Further, the application of these parameters to fluid mixtures and the problems associated with the computation of two-phase choked flows of mixtures has not been treated using the one fluid van der Waals approximation (refs. 6 to 11) for predicting thermophysical properties; the pure-mix problem.

In this paper, we wish to address both the pure-pure and the pure-mix problems in two-phase choked flows using the thermophysical properties codes of references 12 and 10, respectively. It is important to study the fluid mechanics of mixtures as most working fluids are mixtures of varying composition.

#### GOVERNING EQUATIONS

The equations governing homogeneous equilibrium two-phase choked flows are detailed in references 2 and 4. The mass flux is given as equation (1):

$$G^2 = \frac{2}{V^2} \int_p^{P_0} V dp \quad (1)$$

Constraints:

$$G^2 \left( \frac{dV}{dp} \right)_e = 1 \quad (2)$$

$$S(P_0, T_0) = \text{constant} \quad (3)$$

The solution of equation (1) is easy enough if  $V$  is known. The whole problem lies in computing  $V$  subject to constraints 2 and 3. For the simplified pure-pure problem, this is rather straightforward using a thermophysical properties package such as GASP (ref. 12), but can become complex for the pure-mix problem, depending on mixture composition.

In this paper, a reference fluid (0) will be used to determine the thermophysical properties necessary to satisfy equations (1), (2), and (3) for both the pure-pure and the pure-mix problems. The mixture equations, detailed by Mollerup (refs. 7 to 10), are given here in abridged form where  $Z$  is the compressibility function,  $g$  the configurational Gibbs free energy, and  $x_j$  the mole fraction of component  $j$ .

$$Z_m(V, T, x_j) = Z_0(V/h, T/f) \quad (4)$$

$$g_m(V, T, x_j) = fg_0(V/h, T/f) + RT \left( \sum_j x_j \ln x_j - \ln h \right) \quad (5)$$

where the scaling functions,  $f$  and  $h$  are defined as:

$$h = \sum_i \sum_j x_i x_j h_{ij} \quad (6)$$

$$fh = \sum_i \sum_j x_i x_j h_{ij} f_{ij} \quad (7)$$

and the interaction parameters  $h_{ij}$  and  $f_{ij}$  are

defined in terms of assumed mixing rules and critical parameters relating component- $k$  to the reference fluid (0):

$$f_{ij} = n_{ij}(f_{ij}, f_{jj})^{1/2} \quad (8)$$

$$n_{ij} = \phi_{ij} \left( \frac{h_{ii}^{1/3} + h_{jj}^{1/3}}{2} \right)^3 \quad (9)$$

$$f_{ii} = \left( \frac{T_i^c}{T_0^c} \right) \phi; h_{ii} = \left( \frac{V_i^c}{V_0^c} \right) \phi \quad (10)$$

with binary interaction parameters  $n_{ij}$  and  $\phi_{ij}$ . Configuration functions  $\phi$  and  $\psi$  are slowly varying functions of  $V_R$  and  $T_R$  and can be defined in a variety of ways. The most successful are the Leach-Leyland forms (ref. 6), or their modifications such as given by Mollerup (ref. 10) and McCarty (ref. 11)

$$\phi = 1 + (\omega_i - \omega_0)[\omega_1(V_R - \omega_2) - \omega_3(V_R - \omega_4)] \ln T_R \quad (11)$$

$$\begin{aligned} \frac{z_0^c}{z_i^c} \psi = 1 + (\omega_i - \omega_0) & \left[ b_1 - b_2 \ln T_R \right. \\ & \left. + \left( b_3 - \frac{b_4}{T_R} \right) (V_R - b_5) \right] \end{aligned} \quad (12)$$

The coefficients  $a_j$  and  $b_j$  are estimated from experimental data (refs. 10 and 11).

For the pure-pure problem, equations (4) to (10) are simplified since the cross terms do not enter; for example, with only one component, equations (5) to (7) become:

$$g(V, T, 1) = fg_0(V/h, T/f) - RT \ln h \quad (13)$$

$$h = \left( \frac{T^c}{T_0^c} \right) \phi \quad (14)$$

$$f = \left( \frac{V^c}{V_0^c} \right) \phi \quad (15)$$

For the derivatives necessary to solve the governing equations, see Mollerup (ref. 10).

#### RESULTS

The pure-pure problem results are presented first since they are direct and readily explained in terms of data. By contrast, the pure-mix problem which is complex, is further complicated by lack of data.

#### Pure-Pure

Using the thermophysical property codes of reference 12, the governing equations were solved for pure components nitrogen and oxygen on three selected isotherms for which accurate experimental data are available. Subsequent verification checks were made using the Mollerup code, (ref. 10), with simi-

lar results; the exception being near the saturation locus where some discrepancies noted.

In figures 1(a) and (b) the calculated critical mass flux and pressure ratio profiles in normalized coordinates are compared to experimental data. The curve labeled  $\text{CH}_4 - \text{N}_2$  was calculated using the properties of methane, that is, fluid (0) is methane and fluid (a) is nitrogen; similarly, for the curve marked  $\text{CH}_4 - \text{O}_2$ . The use of nitrogen or oxygen as the reference fluid do not alter the results of figures 1 to 3. The agreement with data is quite good, and similar departures from a single curve were found when using fluid nitrogen or fluid oxygen properties directly.

Approaching the critical isotherm, while the mass flux agreement is good, figure 2(a), a rather large and as yet unexplained departure in the pressure profiles between data and theory can be noted, figure 2(b).

Close to the critical isotherm, the agreement with data is again good, as noted in figures 3(a) and (b).

It must be pointed out that the fluid nitrogen and fluid oxygen data are in very good agreement. The discrepancies lie in the governing equations, and their solutions.

#### Pure-Mix

Some initial computations using the governing equations and the more conventional corresponding states approach to defining the normalizing parameters appeared successful. But a closer examination revealed several problems and the approach was abandoned. Calculations for two mixtures are presented as a method of comparison.

Conventional corresponding states techniques, some of which are given in reference 13, cannot be applied to mixtures with any degree of confidence. The linear molar fraction method:

$$t^c = \sum_i t_{ii}^c \quad (16)$$

$$\rho^c = Z^c R T^c / V^c \quad (17)$$

where  $t^c$  represents a property, is simple to apply but not reliable and the complex techniques recommended by reference 14 are better.

With the molar fractions of mixtures  $\text{Mix}_1$  and  $\text{Mix}_2$  given in tables I and II, some estimates of the critical parameters can be made which then can be compared to those estimated using Mollerup's program (ref. 10). The results are given in tables I and II to illustrate the point. Further, the circondenbar (maximum pressure) and circondenthern (maximum temperature) are given for each mixture. For all calculations the reference fluid is methane.

The nature of the vapor pressure locus at a fixed composition is given as figure 4 for mixtures  $\text{Mix}_1$  and  $\text{Mix}_2$ , respectively. While alike in general appearance, the critical point of  $\text{Mix}_2$  is close to the circondenbar. Further note that at temperatures greater than critical, following an isotherm from the high-pressure gas side with decreasing pressure, condensation first occurs on the dew line and attains a maximum density followed by an evaporation at the dew line again, and returns to the low pressure gas state. The composition of the fluid changes, as illustrated in figure 5 for the major components of  $\text{Mix}_1$ . At lower pressures, the

liquid is dominated by the least volatile components n-heptane and hexane. Finally, a temperature entropy diagram, figure 6, for  $\text{Mix}_1$  can be used to "spot" and follow the expansion process. Note that expansions occurring between 190 and 400 K, depending on pressure, terminate at about the saturation locus near the critical point to the circondenthern; that is, the region most difficult to handle and which is the one of most interest.

With this behavior, it should not be too surprising that we have significant difficulties in computing the critical mass flux for  $\text{Mix}_1$  and  $\text{Mix}_2$ .

The critical mass flux for  $\text{Mix}_1$  in normalized coordinates is presented in figure 7 with the conventional pure-pure normalized locii, as background. There are rather significant differences: (1) the saturation locus, (2) the slopes of the isotherms, and (3) regions where computations are incomplete; the exception being the gaseous phase where similar behavior is noted. In many computational attempts, no reasonable solution was found as illustrated by the 1.1 reduced isotherm and the regions previously cited from the near-critical to the circondenthern. These difficulties will require a reassessment of the governing equations.

As a further comparison, the solution of the governing equations for a second similar mixture (both LNG),  $\text{Mix}_2$  was carried out. The results are given in normalized coordinates in figure 8. Comparing the results for  $\text{Mix}_1$  and  $\text{Mix}_2$  indicates two possible similarities: (1) the slopes of the isotherms and (2) the saturation locii are in better agreement than with the pure-pure background curves. Figure 9 gives a more direct comparison between  $\text{Mix}_1$  and  $\text{Mix}_2$  and corresponding states. The  $G^*$  values for  $\text{Mix}_1$  and  $\text{Mix}_2$  were calculated using reference 13. At this time it does not appear reasonable to expect these curves to "collapse" to representative isotherms as composition dependence significantly alters the behavior near the saturation locus. Experimental two-phase choked flow data for fluid mixtures are indispensable.

#### SUMMARY

For the pure-pure problem involving fluids of simple (non-quantum) molecular structure, the conventional corresponding states approach to computations of two-phase choked flows appears valid. The use of the van der Waals one fluid model and a computer program such as Mollerup (ref. 10), with the appropriate reference fluid also appears to be a valid approach.

The departures of two-phase choked flows in normalized coordinates for the pure-pure and the pure-mix problems are significant and composition dependent.

For the mixture, the critical parameters, circondenbar and circondenthern need to be determined from the governing equations or experimental data. Once found, some normalization may be effective in grouping data as it becomes available.

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TABLE I. - MIXTURE COMPOSITION, NORMALIZING AND CRITICAL PARAMETERS FOR MIX<sub>1</sub>

Composition-Mole Fraction

1. Methane	0.9718	5. n-Butane	0.0048	9. Heptane	0.0036
2. Ethane	0.0477	6. i-Pentane	0.0013	10. Nitrogen	0.026
3. Propane	0.017	7. n-Pentane	0.001	11. Carbon dioxide	0.01
4. i-Butane	0.0028	8. Hexane	0.001		

Method	P <sub>c</sub> , MPa	T <sub>c</sub> , K	V <sub>c</sub> , cc/g	Z <sub>c</sub>	m, g/g-mole	G*, g/cm <sup>2</sup> -sec	Circondenbar, MPa	Circondenthem, K
Eq. (16)	4.6	202.7	5.79	0.285	18.02	5280	----	----
Ref. 13	6.21	213.0	5.3	0.335	18.02	5915	----	----
Mollerup code (ref. 10)	6.46	212.0	4.26	0.281	18.02	7340	8.45	267.4

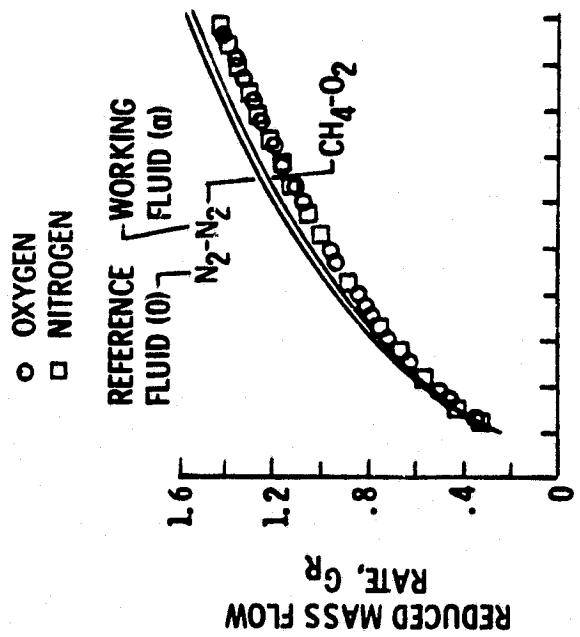
TABLE II. - MIXTURE COMPOSITION, NORMALIZING AND CRITICAL PARAMETERS FOR MIX<sub>2</sub>

Composition-Mole Fraction

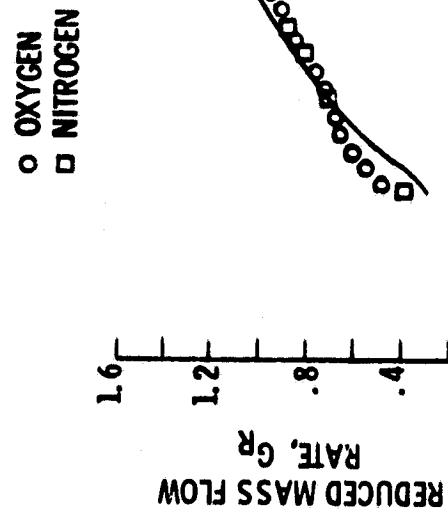
1. Methane	0.6975	3. Propane	0.092	5. n-Butane	0.029
2. Ethane	0.156	4. i-Butane	0.014	6. Nitrogen	0.0115

Method	P <sub>c</sub> , MPa	T <sub>c</sub> , K	V <sub>c</sub> , cc/g	Z <sub>c</sub>	m, g/g-mole	G*, g/cm <sup>2</sup> -sec	Circondenbar, MPa	Circondenthem, K
Eq. (16)	4.53	234.0	5.36	0.284	22.75	5455	---	----
Ref. 13	8.95	261.0	4.39	0.411	22.75	7040	---	----
Mollerup code (ref. 10)	8.9	243.0	3.09	0.309	22.75	9650	9.2	299.0

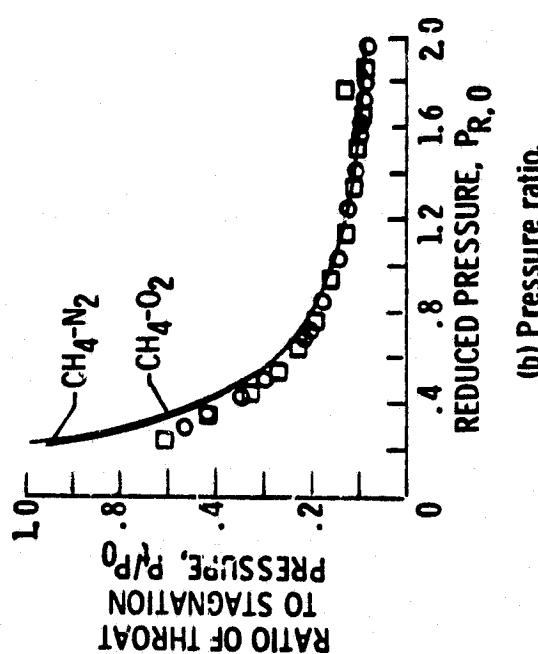
$G^* = \sqrt{P_c V_c / Z_c}$  and  $G_a^* = \sqrt{f/h} G_0^*$  for corresponding states applications with reference fluid (0) and working fluid (a) nearly equivalent for these fluids.



(a) Choked flow rate.

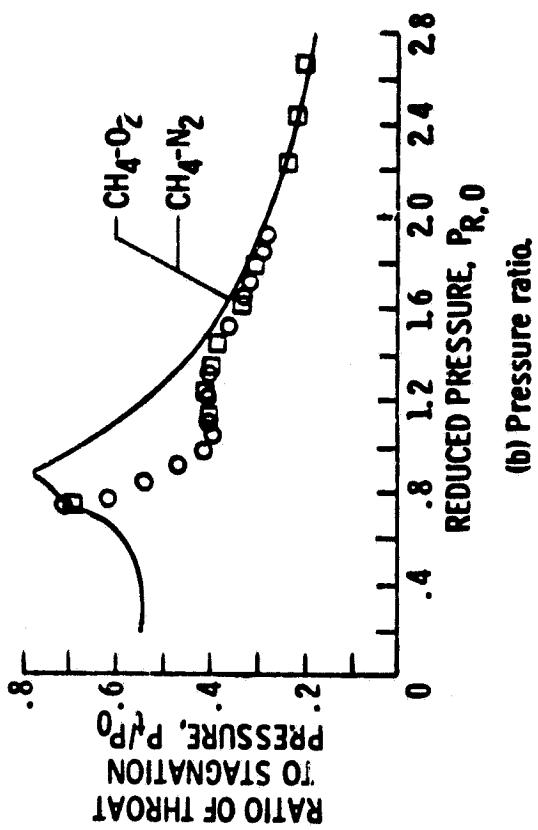


(a) Choked flow rate.



(b) Pressure ratio.

Figure 1. - Choked flow rate and pressure ratio as a function of reduced pressure for a reduced temperature of 0.749 - conical nozzle.



(b) Pressure ratio.

Figure 2. - Choked flow rate and pressure ratio as a function of reduced pressure for a reduced temperature of 0.942 - conical nozzle.

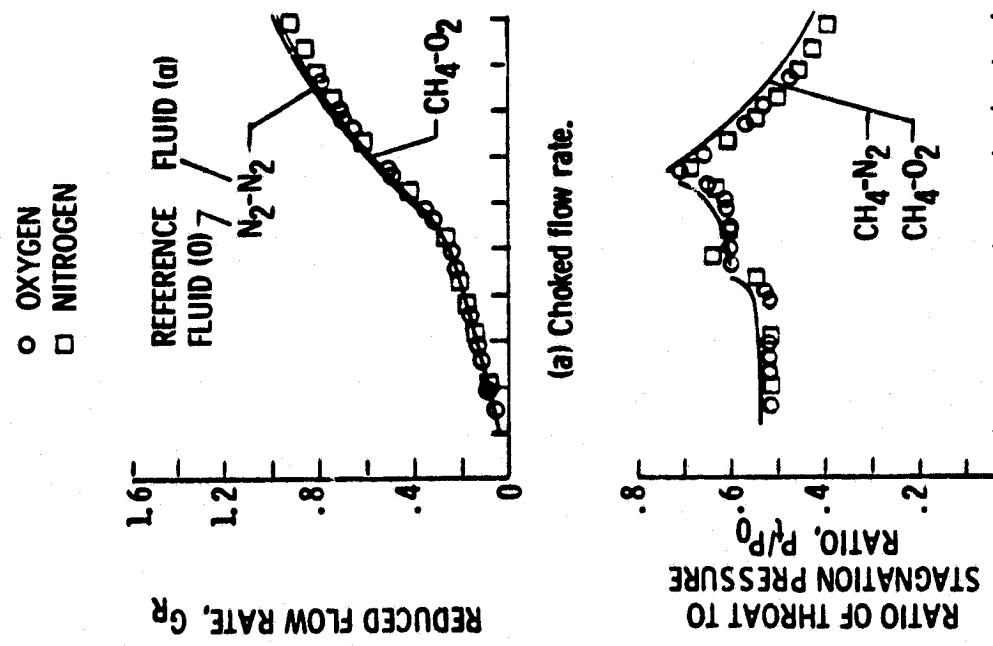


Figure 3. - Choked flow rate and pressure ratio as a function of reduced pressure for a reduced temperature of 1.025 - conical nozzle.

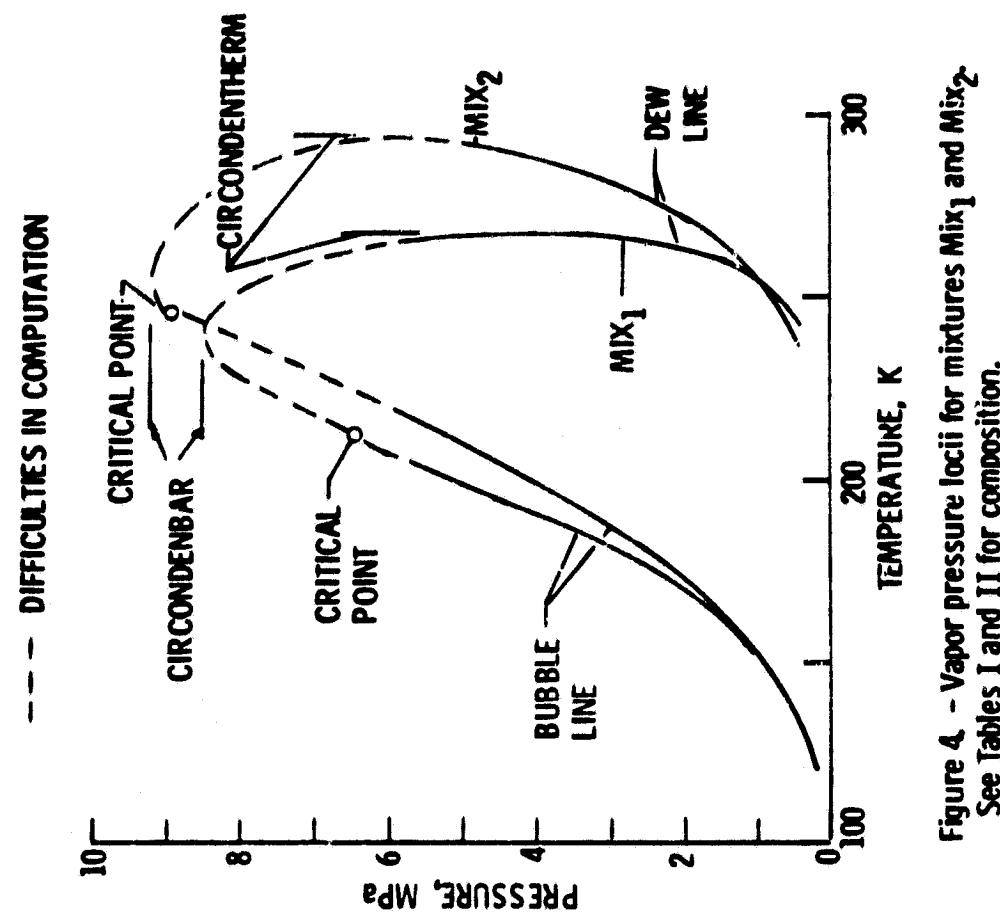


Figure 4. - Vapor pressure locii for mixtures Mix<sub>1</sub> and Mix<sub>2</sub>.  
See Tables I and II for composition.

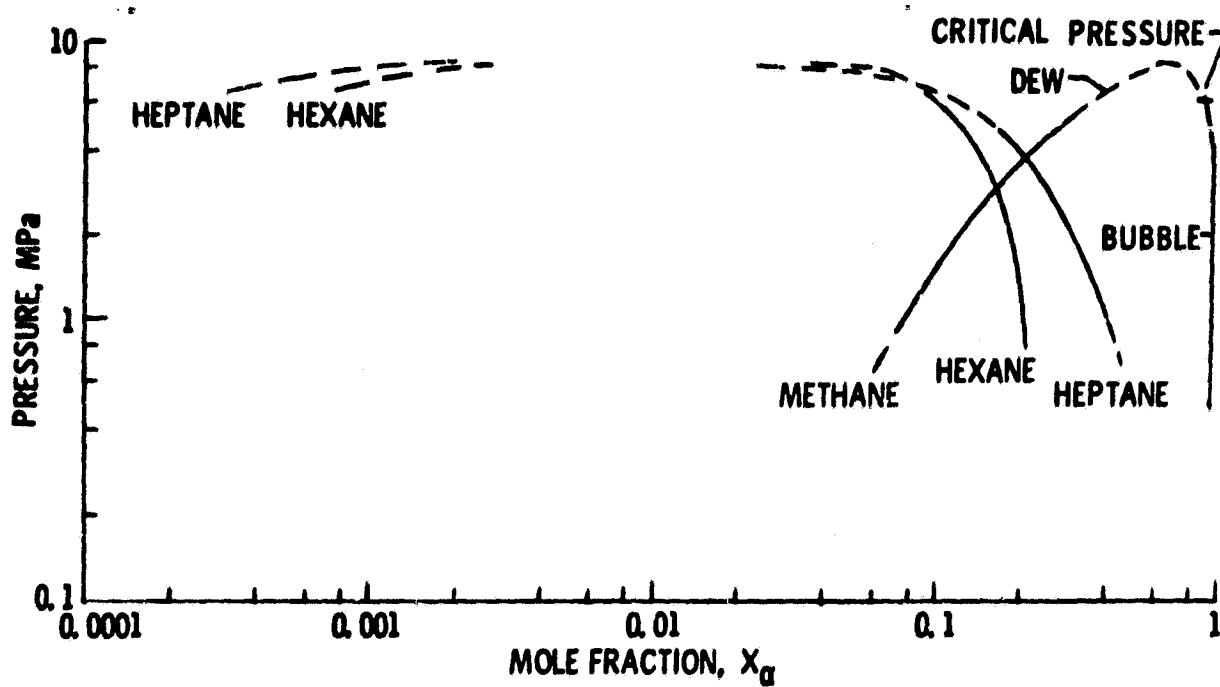


Figure 5. - Primary mole fractions - pressure locii at saturation conditions for mixture Mix<sub>1</sub>. See Table I for complete composition array.

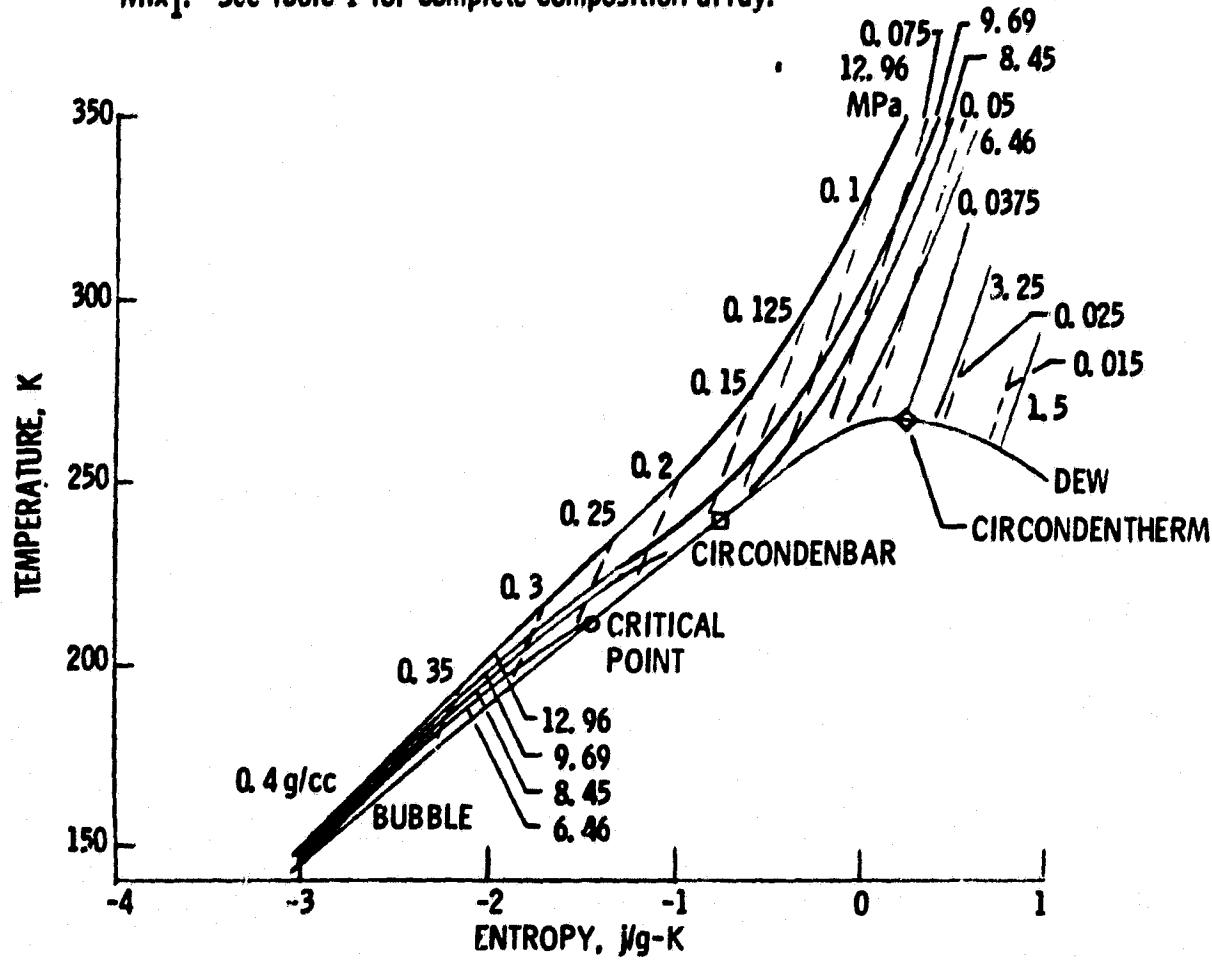


Figure 6. - Temperature - entropy chart for mixture Mix<sub>1</sub>. See Table I for composition.

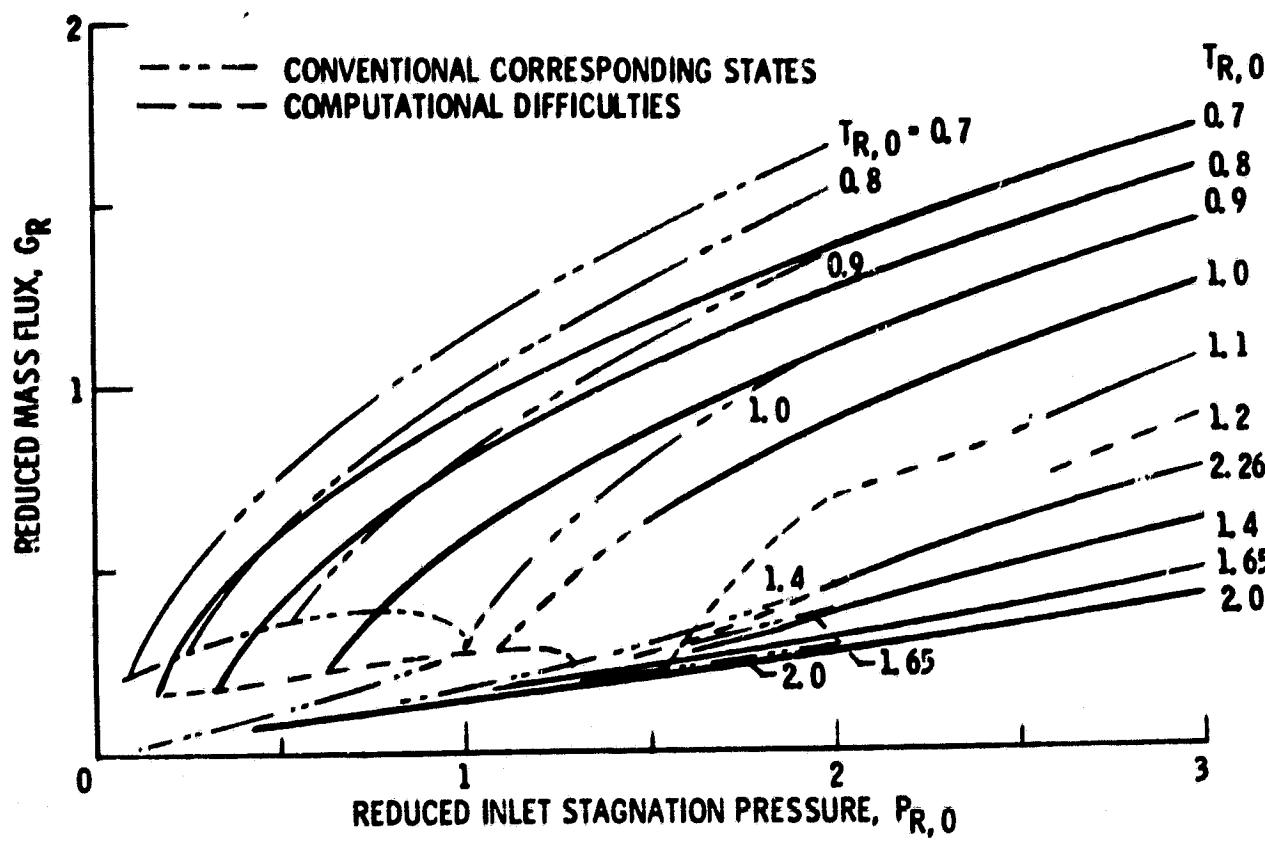


Figure 7. - Reduced critical mass flux as a function of reduced inlet stagnation temperature for selected isotherms for mixture  $\text{Mix}_1$ , with conventional corresponding states locii as background.

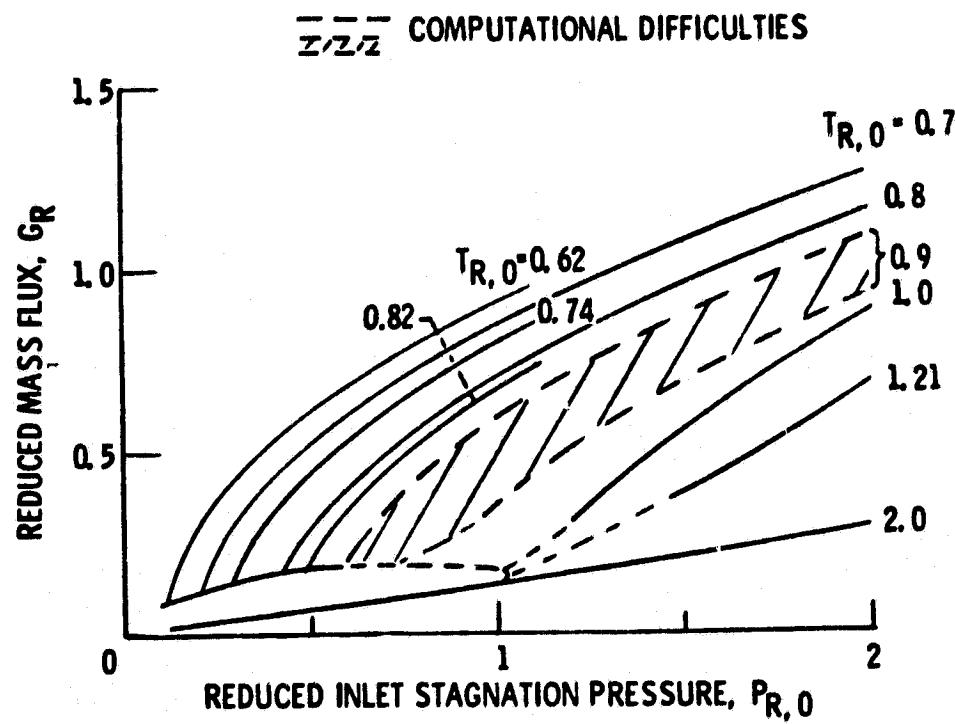


Figure 8. - Reduced critical mass flux as a function of reduced inlet stagnation pressure for selected isotherms for mixture  $\text{Mix}_2$ .

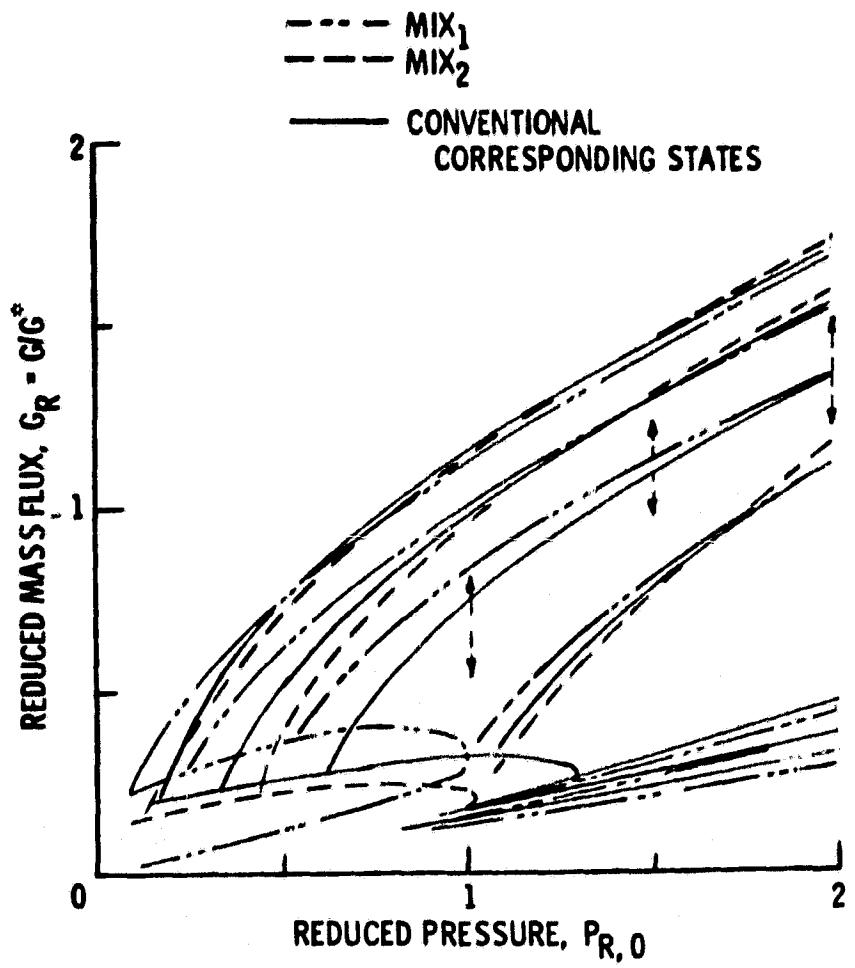


Figure 9. - A comparison of reduced critical mass flux as a function of reduced inlet stagnation pressure for selected isotherms for Mix<sub>1</sub>, Mix<sub>2</sub>, and corresponding states using G\* Tables I, II, ref. 13.

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